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UNC-5157 (Supplement 1)

MODIFICATION OF UNC-SAM-2 TO UNC-SAM-3

by

E.S. Troubetzkoy

January 1970

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DEFENSE ATOMIC SUPPORT AGENCY
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ABSTRACT

This document is a supplement to UNC-5157 and describes the changes in the UNC-SAM-2 programs which have been made to accommodate a revised cross section format. This modified program has been designated UNC-SAM-3.

The Chapter numbers in this document have been assigned to correspond to those of UNC-5157. Chapters 2, 3, 4 and 5 are complete replacements. The material contained in other chapters of this document are additions to the description given in UNC-5157.

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1.3.3 Picking from the Modified Transport Kernel and Scoring of Fluxes

A modification has been introduced in the tracking routine CARLO which does not affect the input. The modification deals with Russian-rouletting of tracks into regions of decreasing importance. As described in Section 1.3.3 of UNC-5157, the decision on whether to terminate or to continue the tracking was based on an independent game of chance. The decision is now based on the random number ξ_1 determining the collision points. This modification corresponds to no change in scoring per track, but to an improvement in the variance associated with the number of selected collision points per track.

2. SHORT DESCRIPTION OF THE CODE

The code system is written in FORTRAN for the Control Data Corporation's (CDC) 1604-A computer. A 32-K core and from two to eight magnetic tapes are required. UNC-SAM-3 is, in reality, a chained series of independent programs which process cross-section and geometry data, do the transport problem, and edit the results. A brief summary of the independent programs contained in UNC-SAM-3 follows. Fig. 2 indicates the information flow in the system.

ENDT

The ENDT program reads the neutron cross-section and distribution data from an ENDF/B data tape and generates a set of point value cross sections, angular distributions for elastic scattering, and energy distribution for secondary neutrons on a variable energy mesh which is established by the program to meet the input-specified criteria for accuracy of representation of the ENDF/B data.

The output of the program is an Element Data Tape (EDT) which contains elemental cross-section data on an energy mesh which is unique for each element, in addition to all the supplemental information required by the UNC-SAM-3 program.

TUNC

TUNC is the main program of an overlay tape. Fig. 3 indicates the information flow in the system. It essentially calls in sequence the following subprograms.

BAND

Given the materials contained in the configuration, an Organized Data Tape (ODT) is created by the BAND routine. The ODT contains the cross sections for the materials used by the problem organized in the required energy band structure.

BEDIT

Edits an existing Organized Data Tape.

GEOM

This is a routine which takes a simplified geometrical description of the physical system, as provided by the problem originator, and produces the rather complex set of data required by the transport program.

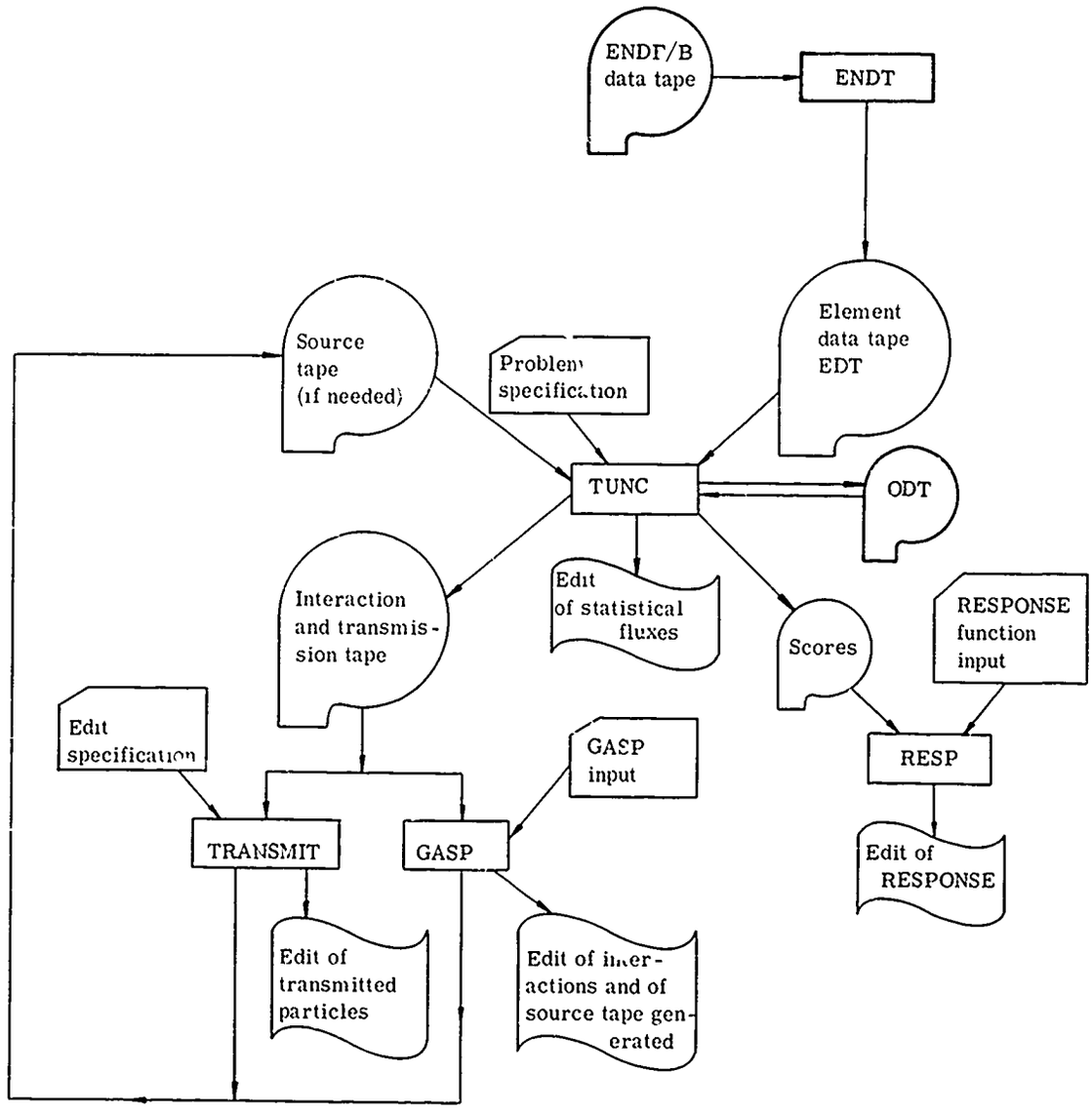


Fig. 2 — UNC-SAM-3 Flow Diagram

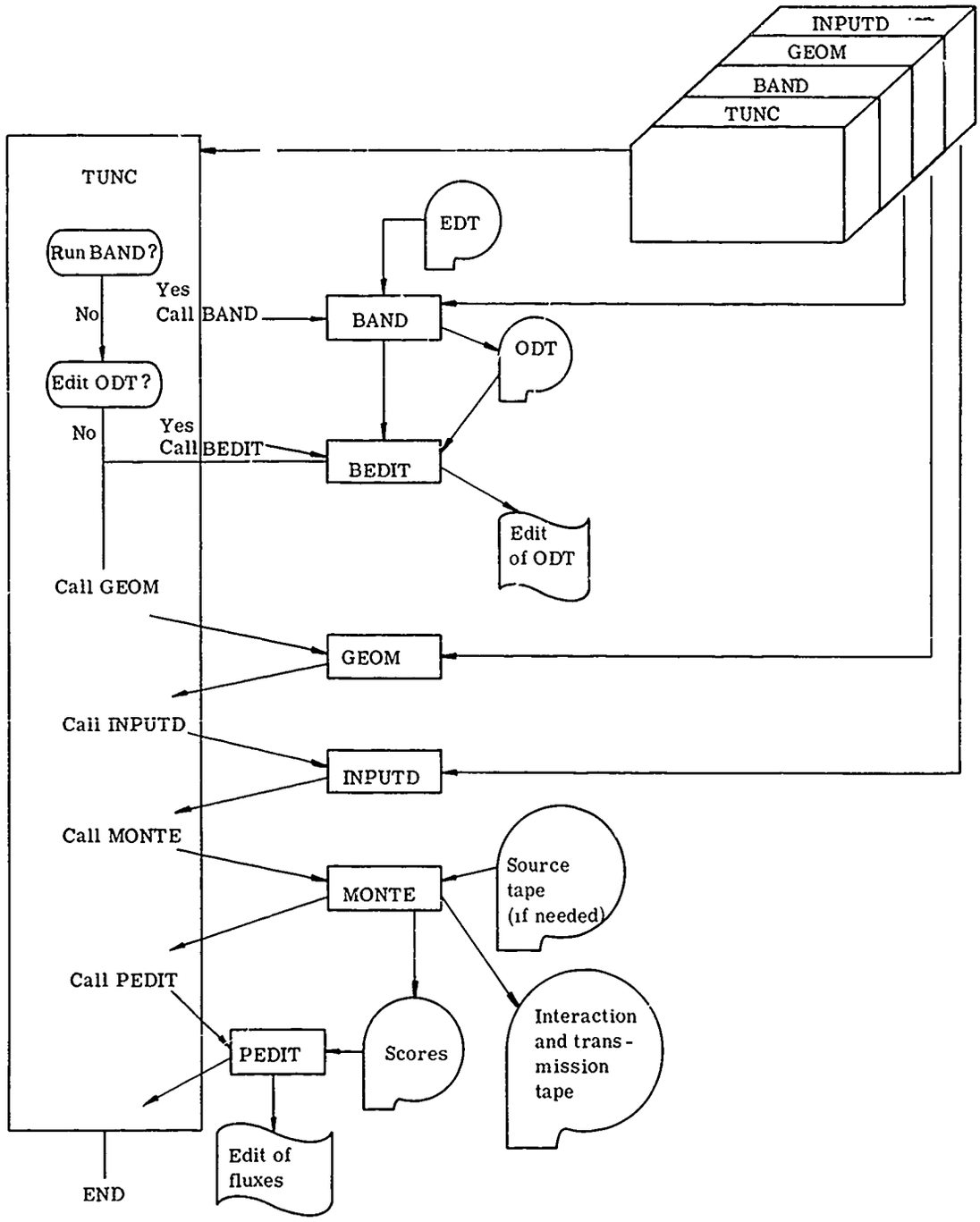


Fig. 3 — TUNC Flow Diagram

Three types of geometries are available: Type 1 is for axially symmetrical problems; Type 2 is for spherically symmetrical problems; and Type 3 is for more complicated geometries, in which case the problem originator must decompose space into a set of boxes known as "ordinary regions." Inside these boxes may be placed "nonordinary regions" consisting of spheres, cylinders, wedges, or other boxes. Nonordinary regions may enclose other nonordinary regions.

INPUTD

Reads in the remaining problem specifications, namely, the assignment of compositions to geometrical regions, the assignment of regions, energy, and angular dependent statistical weights, and the assignment of scoring regions (i.e., regions where average fluxes are to be calculated), as well as the positions of point detectors.

The source specification is also read in. The source can be defined by either an external source tape, or by a description of the energy spectrum and by a power density in different regions.

MONTE

Given the output of the previous subprograms, one is now ready to proceed with the transport program MONTE. The program picks source particles, tracks them to escape (scoring flux contributions where needed), distributing (and storing) collision points. Particles coming out of collision (if any) are subject to the same treatment as source particles. The calculation is done in statistical groups so that variances can be calculated. The energy range is broken up into supergroups to decrease memory limitations. Information (cross sections and scores) relevant to only one supergroup is in the computer memory at any time. Answers for each statistical group and each supergroup are written on a scratch tape.

PEDIT

Reads and edits the output tape of MONTE, giving fluxes and standard deviations.

TRANSMIT

TRANSMIT accepts as input an interaction and transmission tape generated by MONTE. It selects only transmitted particles, i.e., particles which enter a given region during the MONTE tracking, and writes out a source tape consisting of these particles. It also edits that tape.

GASP

The routine Gamma Source Particle generator (GASP) computes gamma-ray production from a primary neutron problem to serve as a source for a secondary gamma-ray problem. GASP requires:

1. An interaction tape (generated by a previous TUNC problem) containing a record of all interactions able to cause gamma-ray emission.
2. Probability numbers for each nuclide of the probable number of gamma rays emitted as a function of energy.

The routine can cope with the generation of other secondaries upon modification of the probability number input. The output of either GASP or TRANSMIT is a source particle tape which becomes input to TUNC.

RESPONSE

This program accepts as input the output tape of MONTE. It calculates integrals $\int R(E)\varphi(E)dE$ and associated statistical errors for specified functions $R(E)$ in specified regions.

3. DATA PROCESSOR ROUTINE (ENDT) AND THE MAIN CODE, TUNC

The ENDT program is described in detail in UNC-5243 (DASA-2337). Nuclide identification is by a five-digit number ZZAAA where ZZ is the atomic number and AAA is the atomic weight. AAA is set to zero for the natural element. In UNC-SAM-3, the n, 2n and other reactions resulting in a secondary neutron are treated through the use of a multiplicity for neutrons following "inelastic" scattering. Beryllium is no longer a special case.

TUNC is the main program of an overlay tape. The input consists of two cards, a title card and a data card containing IBAND and NBAND.

If IBAND = 0	TUNC will call BAND which creates an Organized Data Tape (ODT), and then will call BEDIT which edits the ODT
If IBAND = 1	TUNC will call BEDIT, which edits an existing ODT
If IBAND = 2	TUNC bypasses both BAND and BEDIT, and programs GEOM, INPUTD, MONTE, and PEDIT are called sequentially
If IBAND = -1	TUNC will call BAND and bypass BEDIT.

4. PROGRAM BAND

The purpose of the BAND program is to arrange the cross-section data in an organized fashion for a particular problem.

Different materials present in the configuration are assigned composition numbers ICOMP, from 1 to NCOMP, where NCOMP is the total number of distinct compositions. Each composition is defined by specifying the atomic concentration C and the identifier IT, ID of each of the nuclides that it contains.

For typical problems treated by UNC-SAM-3, the amount of cross-section data for the entire energy range of interest is such that it cannot be fitted into computer memory. To be able to treat such a situation, one has to break up the total energy range, into NBAND "energy bands." The NBAND + 1 band boundaries EBAND must be specified. The number NBAND ($\leq$49) is specified in "TUNC Input" in UNC-5157.

4.1 BAND INPUT

First Card:

(2I10)	NO = problem identification number NCOMP = number of compositions

Next Cards:

(5E14.6)	EBAND (I), I = 1, (NBAND + 1) = energy band limits, ev, in decreasing order

For each composition in sequential order:

First Card:

(10x, I10)	NE = number of distinct nuclides entering the composition ($\leq$20)

For each of the NE nuclides:

One Card:

(2I5, E15.6)	IT = temperature identifier of element ID = element identifier C = concentration (atoms/cm^3 $\times$ 10^{-24})

Additional input consists of the Element Data Tape containing data in the entire energy range for all elements (IT, ID) needed. It must be mounted on

Logical Tape Unit 11. A scratch tape is used on LTU 9. The total number of distinct nuclides should be ≤30.

4.2 BAND OUTPUT

BAND output consists of an organized data tape on LTU 10.

For each band, the organized data are prepared as a single array SIG, with maximum length of 15,000 words.

5. PROGRAM BEDIT

The program BEDIT edits the cross-section data generated by BAND.

The edit is band by band beginning with the highest energy band.

For each band, the information printed includes:

EBLX – low energy limit of the band
LEBAND – memory required to store the band
IDENT – identification number.

This is followed by a recapitulation of the constituents of each composition (by element identifiers and concentrations.)

This is followed by the cross-section data printout element by element.

For each element, the printout includes the total, scattering, and inelastic cross section, and the "excess multiplicity" at each energy meshpoint. It also includes the elastic scattering cross section as calculated from scattering minus inelastic, and the absorption cross section as calculated from total minus scattering. The indices LCHI, LENN, and LPLEV are also given.

For inelastic scattering and excess multiplicity, the printed values correspond to actual data stored for energy meshpoints above threshold, but are printed as "-0" for energy meshpoints below threshold, for which no values are stored. The same applies to the index LPLEV.

Tables of CHI-values, of ENN values, of energy levels, and of cumulative level excitation cross sections are also given at each energy meshpoint where they exist.

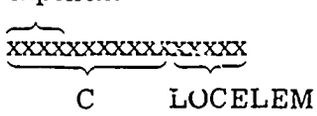
The printout also gives the main pointers of the data. These are labeled by names starting with LOC (e.g., LOCELEM points at the location where data for a particular element starts in the cross-section data array).

The memory layout is as follows:

Location in SIG Array	Description of Contents of SIG
1	$LOCC_{1,1}$ = location of concentration of first element of composition No. 1

Location in SIG Array	Description of Contents of SIG
2	$LOCC_{2,1}$ = location of concentration of first element of composition No. 2
—	—
NCOMP	$LOCC_{NCOMP,1}$ = location of concentration of first element of composition No. NCOMP.
NCOMP + 1	LOCFIRST = 1 + location of concentration of last element of composition No. NCOMP.
$LOCC_{1,1}$ (=NCOMP+2)	Concentration .AND. location* of data (LOCELEM) of 1st element of composition No. 1.
$LOCC_{1,1}+1$	Concentration .AND. location of data of 2nd element of composition No. 1 (if any).
—	—
$LOCC_{2,1}$ - 1	Concentration .AND. location of data of last element of composition No. 1.
—	—
LOCFIRST - 1	Concentration .AND. location of data of last element of composition No. NCOMP.
LOCFIRST	First word of actual data.
LENN = 0	Continuous component of inelastic spectrum is not present.
LENN > 0	The continuous component is described by an ENN table given at location LENN.
LPLEV = 0	Discrete component of inelastic spectrum is not present.
LPLEV > 0	The discrete component is described by a PLEV table given at location LPLEV.

*The notation concentration .AND. LOCELEM means that the floating number representing the concentration has been packed together with the integer LOCELEM: in octal representation on the 48-bit work of the 1604, the packing is as follows:



The remaining (if any) data for the element are laid out as follows:

Location in SIG Array	Description of Contents of SIG
LOCELEV	ELEV (1) = energy levels of target nucleus
—	—
LOCELEV + LEPLEV - 1	ELEV (LEPLEV)
For each LCHI > 5	
LCHI	CHI (1)
—	—
LCHI + LECHI - 1	CHI (LECHI)
For each LENN > 0	
LENN	ENN (1)
—	—
LENN + LEENN -	ENN (LEENN)
For each LPLEV > 0	
LPLEV	PLEV (1)
—	—
LPLEV + LEPLEV - 1	PLEV (LEPLEV)
Finally, for each LOCETAB	
LOCETAB	NETAB = energy table identification number
LOCETAB + 1	LETAB = length of energy table
LOCETAB + 2	ETAB (1) = 1st energy (highest)
—	—
LOCETAB + LETAB + 1	ETAB (LETAB) = last energy (lowest)

Several elements can share the same energy table. All energies are given in ev, all cross sections in barns.

The last word of cross-section data is SIG (LEBAND). LEBAND is the length of the band. The BAND program writes on tape 10 for each band:

LEBAND	Length of band

Location in SIG Array	Description of Contents of SIG
LEBANDMA	Length of largest band up to current one
NCOMP	Number of compositions
NBAND	Number of bands
EBLX	Low energy limit of band
NO	Problem identification number
[SIG (I), I = 1, LEBAND]	Cross-section data

The data are written as a single binary logical record for each band. The bands are arranged in descending order in energy.

The above layout shows that different elements are now specified by different locations LOCELEM in the SIG array. For each element, starting at the corresponding LOCELEM, the data layout is as follows:

Index of SIG Array	Description of Contents of SIG
LOCELEM	LOCETAB = location of energy table at which cross-section data are given
LOCELEM + 1	LOCSIGT = location of total cross-section table
LOCELEM + 2	LOCSIGS = location of scattering cross-section table
LOCELEM + 3	LOCINEL = location of inelastic cross-section table
LOCELEM + 4	LINEL = length of inelastic cross-section table
LOCELEM + 5	LOCMULT = location of multiplicity table
LOCELEM + 6	LMULT = length of multiplicity table
LOCELEM + 7	LOCELEV = location of the energy level table
LOCELEM + 8	LEPLEV = length of the energy level table
LOCELEM + 9	LECHI = length of the CHI-tables
LOCELEM + 10	LEENN = length of the ENN-tables
LOCELEM + 11	ATWT = atomic weight of nuclide

Index of SIG Array	Description of Contents of SIG
LOCELEM + 12	First 24 bits contain IT; last 24 bits, ID
LOCELEM + 13 LOCELEM + 14 LOCELEM + 15	Reserved for future use
LOCSIGT	SIGT (1) .AND. LCHI
—	—
LOCSIGT + LETAB - 1	SIGT (LETAB) .AND. LCHI
LOCSIGS	SIGS (1) .AND. LENN
—	—
LOCSIGS + LETAB - 1	SIGS (LETAB) .AND. LENN
LOCINEL	SIGI (1) .AND. LPLEV
—	—
LOCINEL + LINEL - 1	SIGI (LINEL) .AND. LPLEV
LOCMULT	MULT (1)
—	—
LOCMULT + LMULT - 1	MULT (LMULT)

LCHI, LENN and LPLEV are 5-octal bit integers with the following meaning:

LCHI = 1	Elastic scattering is isotropic in the C.M. system.
LCHI = 2	Same as above, except that the element is hydrogen - special routines to be used.
LCHI = 3, 4	Elastic scattering is isotropic in the lab system.
LCHI = 5	For γ-ray only: Compton scattering.
LCHI > 5	Elastic scattering is anisotropic. The angular distribution is described by a CHI-table given at location LCHI.

7. INPUTD

One additional card of input follows the first one described in UNC-5157.

Format (12I5)

IRT (2) IRT (3) — IRT (10)	Up to nine additional transmission regions may be designated
IWA (=0)	Absorption events (will not) be written on interaction tape
IWA (=1)	Absorption events (will) be written on interaction tape
IWI (=0)	Inelastic events (will not) be written on interaction tape
IWI (=1)	Inelastic events (will) be written on interaction tape
IWE (=0)	Elastic events (will not) be written on interaction tape
IWE (=1)	Elastic events (will) be written on interaction tape

TCUT can be left blank. The time cutoff is determined by the first time-bin boundary.

8.3 CARLO – THE TRACKING AND SCORING ROUTINE

The tracking routine of UNC-SAM-3 needs a rapid access to cross-section data. Several efficient routines have been prepared to look up cross-section data, to pick from the collision kernel, or to evaluate the probability of a given interaction having occurred.

SUBROUTINE DR1

Given the composition number, ICOMP, and the energy, E, the subroutine DR1 interpolates the total cross section for the first nuclide in the composition, computes its contribution to the total macroscopic cross section of the material, and stores that contribution in the first location of a temporary storage array since this information may be needed by the DR3 routine. The routine then performs the same calculation for the second nuclide of the composition, if any, adds this part of the total macroscopic cross section of the mixture to the contribution from the first nuclide, and stores the sum in the second location of the temporary storage array. The procedure is repeated until all nuclides in the composition have been treated. The total macroscopic cross section of the composition also is stored in a second temporary table, as a function of composition number. If the next call of the DR1 routine is at the same energy, the table is examined. If the cross section was previously calculated, it is not recalculated. The temporary tables are erased each time the energy changes.

SUBROUTINE DR3 (Entry point of DR1)

Given the energy and the composition number present during the last call to the DR1 routine, a call to the DR3 routine will pick an interaction event. The first step is a game of chance to decide with which nuclide the interaction occurred.

The next step is to decide whether the interaction was an absorption. If yes, control is returned to the main program.

If a scattering occurred, the routine will pick the energy E′, and, given the direction WB of the incoming particle, will pick the direction WP of the outgoing particle. The multiplicity ULTIP is also determined.

The decision is made on whether the scattering was elastic or inelastic.

In the case of an elastic scattering, the multiplicity is set to one (1). The LCHI indices tabulated at the energy mesh points immediately above and immediately below E are examined. If they are both five (5), a χ-value is determined by a game of chance combined with a linear interpolation between the two CHI-

tables. If one of the LCHI values is five and the other corresponds to isotropicity (LCHI = 1), a χ-value is determined by a game of chance combined with a linear interpolation between the single CHI-table and an isotropic distribution. In both cases, the χ-value is converted to a scattering angle in the center-of-mass system $\cos\theta = 1 - 2\chi$. In the case of LCHI = 1, $\cos\theta$ is picked from a flat distribution. The angle of scattering is then transformed to the lab system, and the energy E' is calculated, using standard collision mechanics. The direction WP is determined by picking a random azimuthal angle.

Whenever LCHI = 3 or 4, E' is set equal to E, and a random direction WP is picked directly.

The case of hydrogen (LCHI = 2) is treated by picking directly the cosine of the angle in the C.M. system. The case LCHI = 5 (Compton scattering of X-rays) is treated by picking the angle of scattering from the Klein-Nishina probability distribution function. A rejection technique devised by H. Kahn* is used.

In the case of inelastic scattering, one first examines the LPLEV indices at mesh points immediately above and immediately below the energy E. If both are zero, scattering must occur via continuum. If at least one is positive, there is a discrete component of the spectrum. The PLEV-tables give the cumulative cross section for level excitation. LPLEV = 0 corresponds to a table with all zero entries. The code, in effect, interpolates between two PLEV-tables to obtain a table at energy E. The inelastic cross section is multiplied by a random number, and the interpolated PLEV-table is searched for the smallest value greater than this product. If the search fails, the excitation is via continuum; if it is successful, the excitation level is determined. The energy is computed as E' = E - ELEV (I). (We assume no difference between lab and C.M. for inelastic scattering.) If E' is positive, a bona fide level excitation took place. If it is negative, we assume that the below-threshold excitation is due only to interpolation in a finite energy mesh. Somewhat arbitrarily, it is assumed that the next lower level is excited and, if no such level exists, that elastic scattering rather than this inelastic scattering occurred.

The case of continuous spectrum is treated by playing a simple game of chance to pick E' from an interpolated ENN table.

In all cases of inelastic scattering, the direction WP is selected at random.

Finally, the test is made whether E is above or below the threshold for multiplicity one (1). If above, the excess multiplicity is interpolated, and the multiplicity is given as 1 + that excess. If E is below the threshold, the multiplicity is set equal to one (1).

*Kahn, H: Application of Monte Carlo, The RAND Corporation, AECU-3159 (1954).

The type of interaction that occurred is transmitted to the tracking code via an index NCDB.

NCDB = 1	Isotropic C.M.
NCDB = 2	Hydrogen scattering
NCDB = 3	Anisotropic C.M.
NCDB = 4	Isotropic lab
NCDB = 5	Klein-Nishina
NCDB = 6	Absorption
NCDB = 7	Inelastic, continuum
NCDB = 8	Inelastic, level

SUBROUTINE GE (Entry point of DR1)

Given a specific type of scattering and with a specific element at energy, E, and a forced angle of scattering, W, a call to GE will determine the probability G of scattering through this angle to have occurred, and the corresponding energy EP.

G is calculated directly from the applicable scattering law. The calculation of EP is via standard collision mechanics in the case of elastic scattering. EP is set equal to the randomly obtained E′ in the case of inelastic scattering.

SUBROUTINE DR1FA

For efficiency purposes, the flux-at-a-point routines call a different set of data retrieval routines. DR1FA is identical to the routine DR1, but calls to DR1FA do not affect quantities stored by DR1.

SUBROUTINE DR3GEFA (Entry point of DR1FA)

This routine is somewhat equivalent to the combination of DR3 and GE.

Given E and ICOMP as for last call of DR1FA, this routine first picks the nuclide with which scattering occurred, then the type of scattering. For elastic scattering, it never picks E′, WP, but immediately calculates the probability G and the energy EP corresponding to the angle of scattering W. For inelastic scattering, the energy EP is selected from the proper distribution and G is set equal to $1/4\pi$ times the multiplicity.

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13. ABSTRACT

This document is a supplement to UNC-5157 and describes the changes in the UNC-SAM-2 programs which have been made to accommodate a revised cross section format. This modified program has been designated UNC-SAM-3.

The Chapter numbers in this document have been assigned to correspond to those of UNC-5157. Chapters 2, 3, 4 and 5 are complete replacements. The material contained in other chapters of this document are additions to the description given in UNC-5157.

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Shielding						
Monte Carlo						
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